4 - 22 Rate Constant Determination in the Reaction of Gold ion with Carbonyl Using Single-Atom Chemistry in Gas Phase*

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The reactions of single gold ion Au^+ with CO and H_2O molecules in gas phase were studied by experiment and calculation. A reaction tube was designed under the steam of the laser sputtering position to destroy the supersonic molecular jet and enhance the collisions between the sputtered metal ions with gas molecules, ensuring the equilibrium reaction conditions. The ionic products were analyzed by a time-of-flight mass spectrometer. The collision temperature in reaction tube was calibrated to 409 K by the reaction of Au^+ ion and H_2O molecules. The contents of ionic products $Au(CO)^+$ and $Au(CO)_2^+$ in the reaction of Au^+ with CO molecules were monitored under different concentrations of CO in precursor gas (Fig. 1). The combination reaction rate constants of single Au^+ ion sequentially with two CO molecules were determined to be $k_1 = 1.1(2) \times 10^{-12}$ cm^3s^{-1} and $k_2 = 4.5(5) \times 10^{-10}$ cm^3s^{-1}. A high-level *ab initial* calculation predicted the geometric structures and binding energies of the ionic products, as well as the pathway and rate constants of the reactions. This is the first time to obtain the rate constant of single-atom reaction of Au^+ ion with CO molecules, and it is essential to study the activation energy of the reaction and provide a reference for understanding the relevant process.

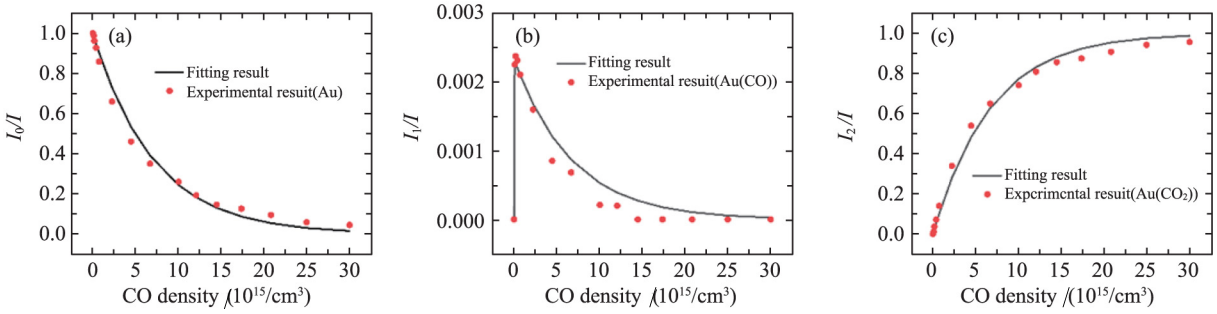

Fig. 1 (color online) Relationship between ionic products and CO concentration. The red dot is the experimental result and the black line is the fitting result.

* Foundation item: National Natural Science Foundation of China (U1832175) and Strategic Priority Research Program of Chinese Academy of Sciences (XDB21030900)